Recent Developments in the Parallelization of Dissipative Particle Dynamics using Shardlow Splitting Algorithms

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Dissipative Particle Dynamics (DPD) is an attractive coarse-graining technique that has become a common method of choice for use in the study of coarsened soft matter. While DPD itself is isothermal, the DPD concepts and methodology have been extended to simulate condensed-phase systems under isothermal, isobaric, isoenergetic, and isoenthalpic conditions. Furthermore, a variant of the isoenergetic approach has recently been developed to model chemical reactivity for coarse-grained models.

While the implementation of these DPD variants is straightforward, the numerical integration of the DPD equations-of-motion is a non-trivial task. In particular, the stochastic component requires special attention due to the pairwise coupling of particles through the random and dissipative forces. The Shardlow-splitting algorithm (SSA) has been found to be the most appropriate integration scheme available to-date and is capable of modeling systems under different fixed condition. Despite significant DPD algorithmic improvements with the SSA, there are considerable challenges in parallelizing the algorithm. In this work, we highlight our recent developments of an efficient parallelization scheme of the SSA and its implementation into LAMMPS. The new capability enables DPD simulations with longer timesteps and improved stability under various fixed conditions.